\* This feff6 input file was generated by Artemis 0.8.012

 \* Atoms written by and copyright (c) Bruce Ravel, 1998-2001

 \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \*

 \* total mu\*x=1: 7.62 microns, unit edge step: 69.75 microns

 \* specific gravity = 16.702

 \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \*

 \* Normalization correction: 0.00030 ang^2

 \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \*

 \* -----------------------------------------------------------------

 \* The following crystallographic data were used:

 \*

 \* title ...

 \* space = F m -3 m

 \* a = 5.4640 b = 5.4640 c = 5.4640

 \* alpha = 90.0 beta = 90.0 gamma = 90.0

 \* core = U edge = L3

 \* atoms

 \* ! elem x y z tag occ

 \* U 1.00000 1.00000 0.00000 U 1.00000

 \* Ce 0.00000 0.00000 0.00000 Ce 1.00000

 \* O 0.25000 0.25000 0.25000 O 1.00000

 \* -----------------------------------------------------------------

 TITLE ...

 HOLE 4 1.0 \* U L3 edge (17166.0 eV), second number is S0^2

 \* mphase,mpath,mfeff,mchi

 CONTROL 1 1 1 1

 PRINT 1 0 0 0

 RMAX 6.0

 \*CRITERIA curved plane

 \*DEBYE temp debye-temp

 NLEG 4

 POTENTIALS

 \* ipot Z element

 0 92 U

 1 92 U

 2 8 O

 ATOMS \* this list contains 75 atoms

 \* x y z ipot tag distance

 0.00000 0.00000 0.00000 0 U\_1 0.00000

 1.36600 1.36600 1.36600 2 O\_1 2.36598

 -1.36600 1.36600 1.36600 2 O\_1 2.36598

 1.36600 -1.36600 1.36600 2 O\_1 2.36598

 -1.36600 -1.36600 1.36600 2 O\_1 2.36598

 1.36600 1.36600 -1.36600 2 O\_1 2.36598

 -1.36600 1.36600 -1.36600 2 O\_1 2.36598

 1.36600 -1.36600 -1.36600 2 O\_1 2.36598

 -1.36600 -1.36600 -1.36600 2 O\_1 2.36598

 2.73200 2.73200 0.00000 1 U\_2 3.86363

 -2.73200 2.73200 0.00000 1 U\_2 3.86363

 2.73200 -2.73200 0.00000 1 U\_2 3.86363

 -2.73200 -2.73200 0.00000 1 U\_2 3.86363

 2.73200 0.00000 2.73200 1 U\_2 3.86363

 -2.73200 0.00000 2.73200 1 U\_2 3.86363

 0.00000 2.73200 2.73200 1 U\_2 3.86363

 0.00000 -2.73200 2.73200 1 U\_2 3.86363

 2.73200 0.00000 -2.73200 1 U\_2 3.86363

 -2.73200 0.00000 -2.73200 1 U\_2 3.86363

 0.00000 2.73200 -2.73200 1 U\_2 3.86363

 0.00000 -2.73200 -2.73200 1 U\_2 3.86363

 4.09800 1.36600 1.36600 2 O\_2 4.53051

 -4.09800 1.36600 1.36600 2 O\_2 4.53051

 1.36600 4.09800 1.36600 2 O\_2 4.53051

 -1.36600 4.09800 1.36600 2 O\_2 4.53051

 4.09800 -1.36600 1.36600 2 O\_2 4.53051

 -4.09800 -1.36600 1.36600 2 O\_2 4.53051

 1.36600 -4.09800 1.36600 2 O\_2 4.53051

 -1.36600 -4.09800 1.36600 2 O\_2 4.53051

 1.36600 1.36600 4.09800 2 O\_2 4.53051

 -1.36600 1.36600 4.09800 2 O\_2 4.53051

 1.36600 -1.36600 4.09800 2 O\_2 4.53051

 -1.36600 -1.36600 4.09800 2 O\_2 4.53051

 4.09800 1.36600 -1.36600 2 O\_2 4.53051

 -4.09800 1.36600 -1.36600 2 O\_2 4.53051

 1.36600 4.09800 -1.36600 2 O\_2 4.53051

 -1.36600 4.09800 -1.36600 2 O\_2 4.53051

 4.09800 -1.36600 -1.36600 2 O\_2 4.53051

 -4.09800 -1.36600 -1.36600 2 O\_2 4.53051

 1.36600 -4.09800 -1.36600 2 O\_2 4.53051

 -1.36600 -4.09800 -1.36600 2 O\_2 4.53051

 1.36600 1.36600 -4.09800 2 O\_2 4.53051

 -1.36600 1.36600 -4.09800 2 O\_2 4.53051

 1.36600 -1.36600 -4.09800 2 O\_2 4.53051

 -1.36600 -1.36600 -4.09800 2 O\_2 4.53051

 5.46400 0.00000 0.00000 1 U\_3 5.46400

 -5.46400 0.00000 0.00000 1 U\_3 5.46400

 0.00000 5.46400 0.00000 1 U\_3 5.46400

 0.00000 -5.46400 0.00000 1 U\_3 5.46400

 0.00000 0.00000 5.46400 1 U\_3 5.46400

 0.00000 0.00000 -5.46400 1 U\_3 5.46400

 4.09800 4.09800 1.36600 2 O\_3 5.95426

 -4.09800 4.09800 1.36600 2 O\_3 5.95426

 4.09800 -4.09800 1.36600 2 O\_3 5.95426

 -4.09800 -4.09800 1.36600 2 O\_3 5.95426

 4.09800 1.36600 4.09800 2 O\_3 5.95426

 -4.09800 1.36600 4.09800 2 O\_3 5.95426

 1.36600 4.09800 4.09800 2 O\_3 5.95426

 -1.36600 4.09800 4.09800 2 O\_3 5.95426

 4.09800 -1.36600 4.09800 2 O\_3 5.95426

 -4.09800 -1.36600 4.09800 2 O\_3 5.95426

 1.36600 -4.09800 4.09800 2 O\_3 5.95426

 -1.36600 -4.09800 4.09800 2 O\_3 5.95426

 4.09800 4.09800 -1.36600 2 O\_3 5.95426

 -4.09800 4.09800 -1.36600 2 O\_3 5.95426

 4.09800 -4.09800 -1.36600 2 O\_3 5.95426

 -4.09800 -4.09800 -1.36600 2 O\_3 5.95426

 4.09800 1.36600 -4.09800 2 O\_3 5.95426

 -4.09800 1.36600 -4.09800 2 O\_3 5.95426

 1.36600 4.09800 -4.09800 2 O\_3 5.95426

 -1.36600 4.09800 -4.09800 2 O\_3 5.95426

 4.09800 -1.36600 -4.09800 2 O\_3 5.95426

 -4.09800 -1.36600 -4.09800 2 O\_3 5.95426

 1.36600 -4.09800 -4.09800 2 O\_3 5.95426

 -1.36600 -4.09800 -4.09800 2 O\_3 5.95426

 END